THEORETICAL STUDY OF M^+—RG_2 (M^+ = CA — RA; RG = HE — RN)

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Ab initio calculations were employed to investigate M^+—RG_2 species. Trends in binding energies, D_e, bond lengths, and bond angles are discussed and rationalised by analysing the electronic wavefunction. Mulliken, natural population, and atoms-in-molecules (AIM) population analyses are performed. It is found that some complexes are linear whereas others are bent. Those results are discussed in terms of hybridization and the various interactions present in these species. The work is a continuation from a previously published study[a] where Group 2 Be^+—RG_2 and Mg^+—RG_2 species are investigated and compared with Group 1 Li^+—RG_2 and Na^+—RG_2 species.

[a] A. Andrejeva, A. M. Gardner, J. B. Graneek, R. J. Plowright, W. H. Breckenridge and T. G. Wright, J. Phys. Chem. A., 117, 13578 (2013)